Participating Institutions

We gratefully acknowledge the funding from
the U.S. Department of Energy Office of Science
Fusion Energy Sciences Program
Grant # DE-SC0001939
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<td><em>A Comparison of Emissive Probe Techniques for Electric Potential Measurements in a Complex Plasma</em></td>
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<td><em>Studies of Fast Ionization Wave Discharges and Development of Sub-Nanosecond Time Resolution Plasma Optical Diagnostics</em></td>
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<td><em>Picosecond CARS Diagnostics for Measurement of Vibrational Distribution Function and Electric Field</em></td>
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<td>12:10 – 12:35</td>
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<td><em>Probe Measurements of Electron Energy Distributions in Plasmas</em></td>
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<td>12:35 – 1:00</td>
<td>Vladimir Kolobov (CFDRC/University of Alabama, Huntsville)</td>
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<td><em>Plasma Simulations with Adaptive Cartesian Mesh</em></td>
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<td>Chi-Shung Yip (University of Wisconsin) <em>Maxwell Demon and Its Instabilities</em></td>
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<td>Cyril Galitzine (University of Michigan) <em>Simulation of Trace Species via DSMC</em></td>
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<td>Michael Campanell (PPPL) <em>Velocity Space Diffusion of Marginally Confined Electrons Driving Sheath Instability and Energy Leaking in E×B Devices with Secondary Emission</em></td>
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<td>Emi Kawamura (University of California, Berkeley) <em>Fluid and Kinetic Simulations of Inductive/Capacitive Electronegative Discharges</em></td>
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| 8:30 – 8:55       | Iain Boyd (University of Michigan)  
*Particle Simulation of Trace Species in a Rarefied Plasma* |
| 8:55 – 9:20       | Mike Lieberman (University of California, Berkeley)  
*Fast Computation of Kinetic Effects in Plasma Processing Discharges* |
| 9:20 – 9:45       | Igor Kaganovich (PPPL)  
*Controlling Plasma Properties in Low-Collisional Plasmas with Active Boundaries* |
| 9:45 – 10:10      | Demetre Economou (University of Houston)  
*Simulation of the Effect of Tailored Bias Voltage Waveforms on the IED* |
| 10:10 – 10:35     | Greg Hebner (SNLA)  
*Laser and Optical Diagnostics of High Voltage Pulsed Plasma Discharges* |
| 10:35 – 10:55     | Coffee Break |
| 10:55 – 12:30 pm  | *Group Discussion* – Collaborations, topics, path forward |
| 12:30 – 2:00      | Lunch (provided); OFES Meeting |
Abstracts: Oral Presentations

MAGNETICALLY INSULATED BAFFLED (MIB) PROBE FOR MAGNETIZED PLASMA DIAGNOSTICS

V. I. Demidov\(^{(a)}\), S. M. Finnegan\(^{(a)}\), M. E. Koepke\(^{(a)}\), Y. Raitses\(^{(b)}\) and S. F. Adams\(^{(c)}\)

\(^{(a)}\) West Virginia University, Morgantown, West Virginia 26506, USA (vldemidov@mail.wvu.edu)
\(^{(b)}\) Princeton Plasma Physics Laboratory, Princeton, New Jersey 08543, USA
\(^{(c)}\) AFRL, Wright-Patterson AFB, Ohio 45433, USA

Measurements of space potentials as well as electron/ion temperatures and densities, and especially their oscillations provide documentation of and insight into basic plasma properties, such as charged particle transport in plasmas. The measurements are particularly vital for fusion related plasmas, but also of great interest for technologically important low-temperature magnetized processing plasmas. For local real-time measurements of the above parameters and their oscillations, various types of electric probes can be used.

In the present work magnetically insulated baffled (MIB) probe clusters have been used for investigation of plasma waves in the steady-state barium plasma column of the West Virginia University Q-machine. The MIB probes have been created by restricting the electron-collection area of a cold Langmuir probe compared to the ion-collection area \([1,2]\). In this case, the probe floating potential can become equal to the space potential, and thus conveniently monitored, rather than to a value shifted from the space potential by an electron-temperature-dependent offset, i.e., the case with an equal-collection-area probe. This design goal is achieved by combining an ambient magnetic field in the plasma with baffles, or shields, on the probe, resulting in species-selective magnetic insulation of the probe collection area. This permits the elimination of electron current to the probe by further adjustment of magnetic insulation which results in an ion-temperature-dependent offset when the probe is electrically floating. Subtracting the floating potential of two magnetically insulated baffled probes, each with a different degree of magnetic insulation, enables the electron or ion temperature to be measured in real time.

The sketch of the used probe construction is shown in Fig. 1. The probe cluster had the following dimensions. Outer radius of the four-bore tube was 1.4 mm and radius of each bore was 0.25 mm. The four-bore tube length was 10 mm. The outer radius of the single-bore tube was 3.2 mm and its inner radius was 1.6 mm. The dimensions of each gap in the outer tube were 2 mm (width) and 5 mm (length). Gold wire with diameter of 0.1 mm, being soft, was used for the collection wire in order to have coil corners that hug the ceramic tube corners. Each coil was created by four windings of gold wire.

A different probe construction has been developed for measurements in NSTX. This work was supported by the DOE OFES (Contract No. DE-SC0001939) and AFOSR.

References

RESULTS FROM A HIGH-SPEED SWEPT LANGMUIR PROBE UNDER DEVELOPMENT

Robert B. Lobbia and Alec D. Gallimore

The University of Michigan, Ann Arbor (lobbia@umich.edu, alec.gallimore@umich.edu)

Given the existence of turbulence and oscillations in many plasma systems, there should be a wide variety of high-speed diagnostic tools to directly measure the constantly varying state of plasma equilibrium. Yet, there exist very few direct high-speed plasma diagnostics. Pulsed and rf plasma systems can employ a host of phase-aligned probe measurements, however, these techniques are severely limited to measuring single oscillation modes with an absence (averaged out) of turbulent features. To overcome these shortcomings, and directly measure the transient state of the plasma—including density, temperature, and energy distribution—the High-speed Dual Langmuir Probe (HDLP) was developed [1,2].

This work is the continuation of ongoing efforts at the University of Michigan to achieve a HDLP temporal measurement resolution of 1-µs. The overall effort is divided into a series of three phases. Phase I (January – May 2010) was focused on testing the base systems and included proof-of-concept trials with commercially available sensors. Phase II (May 2010 – April 2011) entailed a full re-design of all sensors and testing with a 6-kW Hall thruster to acquire vastly improved (over phase I) plasma measurements. In phase III (April – Sept 2011), the diagnostic and methods of analysis will be further refined while making extensive time and space resolved measurements of an 11-kW nested channel Hall thruster. These data will be used to help validate advanced plasma simulation codes in development by collaborating DoE Plasma Science Center (PSC) members. By the end of phase III the fine-tuned diagnostic is expected to attain a readiness level for near real-time in-lab measurement and analysis, facilitating live device optimization in conjunction with thrust or other performance measurements.

Recent results with the HDLP system under continued development include what appear to be the world’s fastest fully swept electrostatic measurements ever performed with a temporal resolution of 2.5 µs (400 kHz). EEDFs were also acquired, but with a temporal resolution of 10 µs due to the smoothing required in applying the Druyvesteyn method. High-speed optical imaging of the discharge was performed synchronously with the HDLP measurements providing a qualitative validation of the identified transients. Ongoing effort to improve the HDLP diagnostic has enabled tremendous gains in sensor sensitivity from 10’s of nA to 100’s of mA with instantaneous dynamic range and bandwidth >100 dB and DC-60 MHz respectively. The developed HDLP is helping unlock the previously hidden realm of time-dependant plasma behavior, providing unique insight into the transient evolution of plasma discharges—aiding both PSC plasma modeling and EEDF control efforts.

References
A COMPARISON OF EMISSIVE PROBE TECHNIQUES FOR ELECTRIC POTENTIAL MEASUREMENTS IN A COMPLEX PLASMA

J. P. Sheehan\(^{(a)}\), Y. Raitses\(^{(b)}\), N. Hershkowitz\(^{(a)}\), I. Kaganovich\(^{(b)}\), and N. J. Fisch\(^{(b)}\)

\(^{(a)}\)University of Wisconsin – Madison (sheehan2@wisc.edu)
\(^{(b)}\)Princeton Plasma Physics Lab

Accurate measurements of the plasma potential are critically important for understanding plasma production, acceleration, and plasma-wall interactions in plasma thrusters. Such measurements are also a critical challenge, especially for complex, flowing, and magnetized plasmas\(^{[1]}\), such as produced in plasma thrusters. Because of its convenience and simplicity, the floating emissive probe technique has been widely employed for potential measurements, especially for Hall thrusters\(^{[2-4]}\). However, this technique is expected to give a measurement of potential \(> T_e/e\) below the plasma potential \((\phi)\) due to space charge effects\(^{[5,6]}\). For plasmas with large \(T_e/\phi\) this may lead to large errors in the determination of the plasma potential profile. We report experimental validation of the predicted space charge effects for the emissive probe. We compare various emissive and non-emissive probe techniques for measuring the plasma potential. The measurements were conducted for a 2kW, 12 cm diameter Hall thruster operated in the Large Thruster Facility at the Princeton Plasma Physics Laboratory (PPPL)\(^{[4]}\). The thruster was operated with xenon gas in a subkilowatt power range and a discharge voltage range of 200 – 450V. The probe was placed at the channel exit where the electron temperature is in the range of 10 to 60eV and the plasma potential is in the range of 50 to 250V. The experimental results generally support theoretical predictions and results of numerical simulations for the potential near the floating electron emitting surface\(^{[7]}\). Specifically, it is shown that the floating potential of the emissive probe is \(\sim 2T_e/e\) below the plasma potential (see Fig. 1). It is observed that the separation technique, which involved measurements of the probe I-V characteristics for cold and hot probes\(^{[8]}\) varies wildly and does not give a good measure of the plasma potential.

References

\(^{[7]}\) Submitted to Physics of Plasmas (March 2011).
CONTROL OF ION ENERGY DISTRIBUTIONS USING A PULSED PLASMA WITH SYNCHRONOUS BIAS ON A BOUNDARY ELECTRODE

H. Shin\textsuperscript{(a)}, V. Donnelly\textsuperscript{(a)}, D. Economou\textsuperscript{(a)}, M. Logue\textsuperscript{(b)}, M. Kushner\textsuperscript{(b)}, D. Graves\textsuperscript{(c)}

\textsuperscript{(a)} Univ. of Houston (economou@uh.edu), (b) Univ. of Michigan, (c) Univ. of California, Berkeley

A retarding field energy analyzer (RFEA) was employed to study ion energy distributions on a grounded substrate in contact with a Faraday-shielded argon inductively coupled plasma (ICP), sustained in a cylindrical discharge tube. \cite{1} Both continuous wave (cw) and power modulated (pulsed) plasmas were investigated. A movable Langmuir probe (LP) was used to measure space- and time-resolved plasma parameters (electron and ion density, electron temperature, plasma potential) along the axis of the discharge tube. For a cw plasma without any bias voltage applied, the IED exhibited a single peak at $V_P$. The peak ion energy decreased with increasing pressure (7-50 mTorr) following the decrease of $V_P$. The single-peaked IED shifted to higher energies by the application of a continuous positive DC bias on a “boundary” electrode in contact with the plasma. The energy shift was controlled by the value of the boundary voltage and followed the change of $V_P$, as measured by the Langmuir probe.

The application of a DC bias on the boundary electrode during a specified time window in the afterglow of a pulsed ICP resulted in a double-peaked IED (Fig. 1). The broader peak corresponds to ions bombarding the substrate during the plasma ON phase of the cycle (no bias), while the sharper peak corresponds to the applied DC bias voltage. By employing such a pulsed plasma and a synchronously pulsed DC bias in the afterglow, the energies of the two peaks as well as their separation, could be precisely controlled. This is important for etching that requires very high selectivity. The full width at half maximum (FWHM) of the sharp peak correlated with the electron temperature in the afterglow.

The FWHM could be made smaller by extending the afterglow duration (smaller duty ratio or smaller plasma power modulation frequency), applying the synchronous DC bias at later times in the afterglow, or extending the time window in the afterglow during which DC bias was applied. All these situations were characterized by lower $T_e$ during the application of DC bias, resulting in smaller FWHM of the respective IED. Ion-neutral collisions, especially in the presheath, and transients in the plasma potential during the application and cessation of the DC bias in the afterglow, could be contributing to the broadening of the IEDs beyond the resolution of the RFEA. A simulation of the experimental reactor was also developed using the Hybrid Plasma Equipment Model (HPEM). IEDs predicted by the simulations were in quantitative agreement with the measurements. We are also collaborating with M. Lieberman of UCB in modeling the resulting IEDs.

\textbf{Reference}

\cite{1} H. Shin et al, submitted to Plasma Sources Science and Technology.

![Fig. 1: IEDs for different pressures under pulsed plasma conditions with a synchronous +24.4 V bias applied on the boundary electrode in the afterglow, over the time window, $\Delta t_b=45-95$ µs. Other conditions: 10 kHz plasma modulation frequency at 20% duty cycle, 120 W average power and 40 sccm argon gas flow.](image-url)
STUDIES OF FAST IONIZATION WAVE DISCHARGES AND DEVELOPMENT OF SUB-NANOSECOND TIME RESOLUTION PLASMA OPTICAL DIAGNOSTICS

I.V. Adamovich, W.R. Lempert, A. Montello and K. Takashima

Dept. of Mechanical and Aerospace Engineering, The Ohio State University
(adamovich.1@osu.edu, lempert.1@osu.edu, montello.5@osu.edu, takashima.6@osu.edu)

Fast Ionization Wave (FIW), nanosecond pulse discharge propagation in nitrogen and helium in a rectangular geometry channel / waveguide is studied experimentally using calibrated capacitive probe measurements. The repetitive nanosecond pulse discharge in the channel was generated using a custom designed pulsed plasma generator (peak voltage 10-40 kV, pulse duration 30-100 nsec, voltage rise time ~1 kV/nsec), generating a sequence of alternating polarity high-voltage pulses at a pulse repetition rate of 20 Hz. Both negative polarity and positive polarity ionization waves have been studied. Ionization wave speed, as well as time-resolved potential distributions and axial electric field distributions in the propagating discharge are inferred from the capacitive probe data. ICCD images show that at the present conditions the FIW discharge in helium is diffuse and volume-filling, while in nitrogen the discharge propagates along the walls of the channel. FIW discharge propagation has been analyzed numerically using quasi-one-dimensional and two-dimensional kinetic models in a hydrodynamic (drift-diffusion), local ionization approximation. The wave speed and the electric field distribution in the wave front predicted by the model are in good agreement with the experimental results (see Fig. 1). A self-similar analytic solution of the fast ionization wave propagation equations has also been obtained. The analytic model of the FIW discharge predicts key ionization wave parameters, such as wave speed, peak electric field in the front, potential difference across the wave, and electron density as functions of the waveform on the high voltage electrode, in good agreement with the numerical calculations and the experimental results.

A brief description of two projects which center on the use of picosecond Coherent Anti-Stokes Raman Spectroscopy (CARS) will also be presented. The first project is a study of vibrational energy loading and relaxation in high pressure non-equilibrium nitrogen plasmas, including a new measurement of the $\text{N}_2 - \text{H}_2$ V-T relaxation rate at 400 K. The second project is the development of an $\text{H}_2$-based CARS diagnostic for non-invasive measurement of spatially resolved electric field with sub nanosecond temporal resolution.

Fig. 1: Comparison of (a) experimental and (b) predicted time-resolved axial electric field at different distances from the high-voltage electrode ($\text{N}_2$, $P=10$ torr, $U=28$ kV, positive polarity wave).

![Fig. 1](image1.png)

Fig. 2: Comparison of numerical solution and self-similar analytic solution for (a) electron density, and (b) axial electric field in the wave front in nitrogen, at $P=10$ torr and $V=1$ cm/nsec (positive polarity wave).

![Fig. 2](image2.png)
PICOSECOND CARS DIAGNOSTICS FOR MEASUREMENT OF VIBRATIONAL DISTRIBUTION FUNCTION AND ELECTRIC FIELD

Aaron Montello\(^{(a)}\), Ben Goldberg\(^{(a)}\), Munetake Nishihara\(^{(a)}\), Igor V. Adamovich\(^{(a)}\), Walter R. Lempert\(^{(a)}\) and Sean O’Byrne\(^{(b)}\)

\(^{(a)}\) The Ohio State University (aaron.montello@gmail.com)
\(^{(b)}\) University of New South Wales, ADFA

We describe the design and implementation of a picosecond CARS diagnostic system, used for measurements of the vibrational distribution function in a nitrogen flow vibrationally excited in a high-pressure electric discharge in the plenum of a nonequilibrium hypersonic wind tunnel. The high-pressure discharge used for vibrational excitation of the flow is a combination of two fully overlapping transverse discharges, a repetitive nanosecond pulse discharge producing volume ionization and a DC discharge used for energy loading. It is shown that the CARS system, using a picosecond Nd:YAG laser and a picosecond modeless broadband dye laser, generates sufficient peak power to acquire single shot spectra with high signal to noise.

The work presented here demonstrates the feasibility of sustaining high vibrational temperatures in a pulser-sustainer discharge in nitrogen, up to \(T_v(N_2)\approx2000\) K, at nearly half atmospheric pressure and at steady state. Previous results, utilizing nitrogen UV/visible emission spectroscopy, have indicated low translational-rotational temperatures at these conditions, \(T=350-400\) K. This demonstrates highly nonequilibrium conditions created by the discharge pair in the nozzle plenum. In addition it is shown that the repetitive nanosecond pulse discharge operating alone also produces vibrational excitation of nitrogen, with vibrational temperatures of up to \(T_v(N_2) = 1100\) K. As expected, vibrational temperature increases with increasing DC voltage, more specifically with increased electric field, \(E/n\). At \(E/n=18\) Td, vibrational temperatures of \(T_v(N_2)=2000\) K are achieved at both discharge pressures.

Nitrogen vibrational temperatures are also reported upon injection of a variety of “relaxer” species. The results demonstrate that injection of oxygen, up to 14% mole fraction, does not result in detectable change of nitrogen vibrational temperature, indicating extremely slow V-V energy transfer from \(N_2\) to \(O_2\), as well as slow \(N_2-O_2\) V-T relaxation at the present conditions. On the other hand, injection of even small amounts of \(CO_2\) (less than 1% mole fraction) results in dramatic \(N_2\) vibrational temperature reduction, due to rapid V-V energy transfer from nitrogen to the asymmetric stretch vibrational mode of \(CO_2\), with subsequent V-T relaxation of \(CO_2\). Injection of \(NO\) or \(H_2\) represents an intermediate case. It is shown, however, that relaxation experiments yield an estimated low temperature \(N_2-H_2\) V-T relaxation rate of approximately \(1\cdot10^{-15}\), an order of magnitude faster than predicted by extrapolation of previously published high temperature shock tube data.

Additionally, progress towards the development of an electric field measurement by picosecond four wave mixing, similar to Coherent Anti-Stokes Raman Spectroscopy (CARS), in a hydrogen discharge with sub-nanosecond time resolution will be presented. It is shown that efficient Raman pumping can be achieved using a stimulated Raman shifting cell to generate the “Stokes” laser beam from the picosecond Nd:YAG pump/probe beam. Conversion efficiency as high as \(\approx30\%\) is shown at a Raman shifting cell pressure of 8 bar. Electric field sensitivity of several tens of volts is ultimately anticipated at 1 Bar pressure.
Fast ionization waves (FIWs) generated by nanosecond, high voltage pulses are important for applications ranging from plasma-assisted combustion and material processing to biomedical treatments. A numerical study of ionization waves, with comparison to experiments, has been conducted using nonPDPSIM, a 2-dimensional plasma hydrodynamics model with radiation photon transport. The investigation addressed three contexts:

1. Study of the fundamental properties of FIWs in moderate pressure dielectric channels to quantify propagation mechanisms. (See Fig. 1.) The FIWs are generated by 48 ns FWHM voltage pulses in N₂ at 10 Torr. Experimental measurements of transient electric fields are used for validation. Peak electron temperatures in the ionization front reach 15 eV with propagation speeds of up to 1 cm/ns. The shape of the ionization front is sensitive to secondary processes on the surface (e.g., photoelectron production).

2. Propagation of FIW in circuitous tubes. Long (≥ 1 m) tubes of less than a few mm diameter are used to deliver plasmas at atmospheric pressure to remote sites. Scaling laws developed in the initial study are used to investigate propagation of FIW in these structures that can have aspect ratios of up to 1000. We find that the curvature of the tube and placement of ground planes can affect the trajectory of the FIW in the tube.

3. Intersection of FIW with surfaces. When a FIW strikes a surface, the majority of the applied potential can be transferred to the transient sheath at the surface, producing surprisingly large ion energies. The ion energy and angular distributions (IEADs) are initially thermal and can spike to energies of tens of eV (See Fig. 2.). The manner of controlling these IEADs by control of the FIW and the subsurface dielectric properties will be discussed.
An electric-probe method for diagnostics of electron energy distribution functions (EEDF) in plasmas is reviewed with emphasis on obtaining reliable results while taking into account appropriate probe construction, various measurement errors and the limitations of probe theories. The starting point is a discussion of the Druyvesteyn method for EEDF measurements in weakly ionized, low-pressure and isotropic plasma. Four major problems in implementing meaningful probe diagnostics in rf plasma reactors are discussed. They are: a) large frequency spectrum with significant amplitudes of the rf plasma rf potential corresponding to source and bias fundamental frequencies and their harmonics; b) low frequency noise due to plasma instability and ripples in an rf power source, c) too high impedance between the plasma and grounded chamber due to limited surface of the chamber and its contamination or/and an artificial protective coating, and d) contamination of the probe surface with a low conductive layer of the reaction products. The probe characteristic distortion caused by these factors are hardly recognized when one just follows Langmuir procedure to infer plasma parameters assuming Maxwellian EEDF, since distorted and undistorted probe characteristics look similarly. But the problem becomes apparent after double differentiation of the distorted probe characteristics (to infer the EEDF) due to error augmentation inherent to differentiation procedure. Design of the probe diagnostic experiment addressing the aforementioned problems is discussed and examples of EEDF measurements with high energy resolution (small fraction of T_e) and large dynamic range (3-4 orders of magnitude) in laboratory and industrial rf plasmas, are given in this presentation.

At present, the Druyvesteyn method is the most developed and routine method of plasma diagnostics. The following section of the review describes an extension of the classical electron distribution measurements to higher pressures, magnetic fields and anisotropic plasmas. Today, these methods have been used by a very limited number of researchers. Their verification has not yet been fully completed, and their reliable implementation still requires additional research. Nevertheless, the described methods are complemented by appropriate examples of measurements demonstrating their potential value.
PLASMA SIMULATIONS WITH ADAPTIVE CARTESIAN MESH

Vladimir Kolobov\textsuperscript{(a)}, Robert Arslanbekov \textsuperscript{(a)} and Gary Zank \textsuperscript{(b)}

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Many problems of plasma physics are characterized by the presence of large gradients of plasma parameters in localized domains (streamers, filaments, ionization fronts, etc). For such problems, the ability to dynamically adapt the local mesh resolution can substantially increase the accuracy and efficiency of simulations. We will describe our new plasma simulation tool with Adaptive Mesh Refinement (AMR) using octree Cartesian mesh. We have already demonstrated our approach for simulation of streamer development with a minimal plasma model (Poisson solver, drift-diffusion electron transport, immobile ions, and local field ionization) \cite{1}. Recently, we developed new capabilities including ion drift, electron energy balance, and simple external circuit \cite{2}.

Having added ion transport to the minimal plasma model, we simulated low-pressure discharges controlled by ion drift to the walls. We have illustrated that fluid model with account for electron thermal conductivity can reproduce qualitatively the complicated structure of the cathode region in DC discharges observed in experiments. In particular, the nonmonotonic distribution of the electrostatic potential was formed with two field reversals in the plasma region and a sharp maximum of plasma density in the vicinity of the first field reversal near the cathode sheath. The electron temperature reached a minimum in the Faraday Dark Space, near the second field reversal. Careful examination shows deficiencies of the fluid model, which operates in terms of an “average electron” and cannot describe the complicated structure of the electron energy distribution function observed in the cathode region. After all, we have shown that fluid plasma models previously developed for the traditional meshing techniques can be extended for the adaptive Cartesian mesh \cite{3}.

The new tool has been applied to studies of microplasmas. Figure 1 illustrates dynamics of gas breakdown between two wires of radius 100 nm separated by a 1 \(\mu\m) distance. A voltage of amplitude 0.2-4 kV was applied between the wires to initiate a pulsed breakdown induced by field emission of electrons from the cathode. The dynamics of gas breakdown were studied using dynamically adaptive Cartesian mesh to resolve the propagation of fast ionization front (illustrated in Figure 1). New physics learned by using the new AMR code will be discussed. We will also describe some computational issues including parallel computations with dynamic load balancing among processors.

References
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THE ROLE OF ATOMIC HYDROGEN ON PLASMA SYNTHESIS OF CARBON NANOTUBES

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Hydrogen containing discharges are used widely in plasma synthesis of a variety of nanostructures including nanoparticles and carbon nanotubes. We developed a method for measuring the H-atom flux at the plane of the substrate surface during H2 plasma exposure. Our method is based on infrared measurements of the change in free-electron absorption in a polycrystalline ZnO film when this film exposed to H atoms. Hydrogen acts as an electron donor in ZnO, and thus the concentration of hydrogen-generated free carriers can be extracted from their absorption in the infrared. The change in the concentration of free carriers can in turn be related to the flux of H atoms impinging on a ZnO film placed on the substrate platen. Using this and a suite of additional plasma and material characterization techniques, including optical emission, infrared, and Raman spectroscopy and electron microscopy we systematically investigated the interrelation among plasma gas phase composition, catalysts morphology, catalyst structure, and carbon nanotube structure in plasma enhanced chemical vapor deposition of carbon nanotubes. The structures of carbon nanotubes grown from catalytic nanoparticles via PECVD in CH4 /H2 mixtures show a strong dependence on the H2-to-CH4 ratio in the feed gas. Hydrogen plays a critical role in determining the final carbon nanotube structure through its effect on the catalyst crystal structure and morphology. At low H2-to-CH4 ratios, iron catalyst nanoparticles are converted to Fe3C and well-graphitized nanotubes grow from elongated Fe3C nanoparticles. High H2-to-CH4 ratios in the feed gas result in high atomic hydrogen concentrations in the plasma and strongly reducing conditions, which prevents conversion of Fe to Fe3C. In the latter case, poorly-graphitized nanofibers grow from ductile bcc iron nanocrystals that are easily deformed into tapered nanocrystals that yield nanotubes with thick walls. In the limit of pure hydrogen the cylindrical pressure walls of a nanotube are etched and amorphized by the H atoms. Etching is not uniform across the length of the CNT but rather, small etch pits form at defective sites on the CNT walls along the entire nanotube length. Once an etch pit is formed, etching proceeds rapidly, and the remainder of the CNT is quickly etched away.
PLASMA-SURFACE INTERACTIONS, EROSION, AND IMPACT ON PLASMA DISTRIBUTION FUNCTIONS: H₂/Ar PLASMA/α-C:H

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The goal of this project is to establish the role of surface processes in influencing/controlling characteristic plasma distributions functions. To understand how the surface influences the plasma distribution functions, we first characterized the plasma modification of the surface. We investigated the surface modification of a-C:H by varying plasma chemistries (Ar, H₂, Ar/H₂) and ion energies (up to 200 eV). Multilayer models for steady-state modified surface layers are constructed using ellipsometric data and compared with results of molecular dynamics (MD) simulations and transport of ions in matter (TRIM) calculations. We find that Ar plasma causes a modified layer at the surface that is depleted of H atoms. This depletion saturates quickly during plasma exposure (< 1 s) and persists during steady-state erosion. We find that the thickness and density of the H-depleted layer are in good agreement with MD and TRIM simulations. The resulting surface modification thicknesses are seen in Fig. 1. The degree of surface densification decreases when small additions of H₂ are added to Ar plasmas. When more than 5% H₂ is added to the plasma, long term loss in surface density is observed, indicating rehydrogenation and saturation of H in the film. As H₂ fraction in plasma increases, the plasma density and ion bombardment of the surface decreases, causing incorporation of H deeper into the a-C:H surface.

The effects of gas mixtures and surface generated carbon on plasma parameters (T_e, plasma density, EEDF) have been explored with Langmuir probe measurements. Fig. 2 shows the change in the EEDF when H₂ gas is flowed into an Ar plasma. At the pressures explored (5-100 mTorr), the plasma density decreases greatly with only small H₂ additions. At high H₂ flows, the electron energy distribution transitions from Maxwellian to Druyvesteyn. The addition of 1-20 % CH₄ into H₂ plasma shows an increase in plasma density and electron temperature. The erosion products of a-C:H films in H₂ plasma are volatile hydrocarbons (CₓHₓ) and we find that they cause a similar effect on plasma properties as CH₄ addition. This observation could be important for controlling plasmas that are used for or experience erosion of different hydrocarbon materials (polymers, graphite). The effect of plasma mixtures and impurities on high energy photon (VUV) emission from the plasma is currently under way.

References
MD SIMULATIONS AND EXPERIMENTS: INTERACTIONS OF α-C:H WITH ARGON AND HYDROGEN PLASMAS

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We studied the interactions of α-C:H and α-C surfaces with ions and radicals typically found in Ar and H\(_2\) plasmas by comparing using molecular dynamic (MD) simulations and \textit{in situ} ellipsometric measurements during experimental exposures. [1,2] The present talk will focus on the results from MD simulations; related talks and posters will detail comparisons between the simulations and experiments. We employ MD simulations based on reactive empirical bond order (REBO) potentials. The major question facing any analysis of plasma-surface interactions and the resultant effects of surface processes on plasma properties such as the distribution functions involves the ways in which the plasma alters the near-surface region. The region within about 2-10 nm from the surface will have its composition and structure (e.g. material density) altered through coupling with plasma species. Ions impacting the surface are generally the most energetic and often play a central role, but neutral radicals and even ultraviolet (uv) photons can be important in some cases. Figure 1 illustrates the H-depleting effects of Ar\(^+\) ions on α-C:H films.

![Image of a-C:H layer before and after Ar\(^+\) ion impacts.](image.png)

The effects of H-containing plasmas on α-C:H surfaces were studied by simulating H\(_2^+\) impacts at normal incidence for a variety of energies. The major reactions are: H insertion; H-depletion; and hydrocarbon cluster erosion. The near-surface film structure and composition under steady state conditions is a result of a competition between erosion and insertion processes. The insertion of hydrogen into the surface during H\(_2^+\) impacts causes expansion of the film due to the polymerization and corresponding reduction in density. At steady state, the modified near-surface layer has a C:H ratio of \(\sim 1\) and thickness \(\sim 2.5\) nm. Interestingly, the same modified layer was observed with H\(_2^+\) impacts on a film with no H originally. We conclude that the modified layer thickness and composition does not depend on the initial surface composition. It does depend on ion and neutral species composition and energy. The experimental value of the modified layer thickness based on ellipsometry is found to be apparently deeper than the MD simulation predictions. We plan to explore the effect of H\(^+\) impacts and synergetic effects of ion and VUV photons.

\textbf{References}


NANOPARTICLE CHARGING IN COLLISIONAL MULTI-COMPONENT PLASMAS

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Particle charging in dusty plasmas has been extensively simulated [1]. Earlier works have assumed the interaction of dust particles with one type of ion in the neutral gas. Our aim is to study particle charging in a plasma environment consisting of multiple types of ions, to determine the effect of different ratios of ion mixtures. A discharge formed in a mixture of two gases whose ionization potentials are close would consist of ions of both the gases. A good example is an argon-hydrogen rf discharge. A mixture of $Ar:H_2:SiH_4$ used for producing silicon nanoparticles in an rf discharge consists of argon and hydrogen ions along with the silicon dust particles [2]. Even in $Ar:SiH_4$ plasmas, hydrogen gas released as a result of the formation of silicon particles can be expected to be ionized. To model multicomponent plasmas we assumed a mixture of $Ar^+$ ions (the most prominent argon ions) and $H_3^+$ ions (the most prominent hydrogen ions at intermediate pressures) in argon gas. We calculated the particle potential analytically and compared it with MC-MD (Monte-Carlo and molecular dynamic) simulations. Figure 1 compares the surface potential that a 200 nm diameter particle experiences in $1 \times 10^{16} m^{-3}$ $Ar^+$ ion density in Ar gas, with that in plasma consisting of an ion mixture of $5 \times 10^{15} m^{-3} Ar^+$ and $5 \times 10^{15} m^{-3} H_3^+$ ions in argon gas. The effective electron temperature was taken to be 3.5 eV, the gas temperature 290 K. The case of $Ar^+$ ions in argon gas shows that in the low pressure regions (up to 1 Pa), the particle potential can be predicted by the OML theory. At intermediate pressures, there is a drop in the potential because of $Ar^+$ ion current is enhanced by collisions. At higher pressures (above 1000 Pa), the ion current to the particle is inhibited due to excessive collisions with neutral gas, causing an increase in the potential. In the case of $Ar^+$ and $H_3^+$ ion mixture, there is an increase in the total current to the particle at low pressures compared to the pure $Ar^+$ case, despite the total ion density being the same. At intermediate pressures, the potential is comparable because the ion current is dominated by the collision enhanced $Ar^+$ current. At higher pressures, however, the particle potential continues to remain low because of the collision enhanced $H_3^+$ current.

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References
THE SPATIOTEMPORAL EVOLUTION OF A NANODUSTY PLASMA: COMPARISON OF MODELING AND EXPERIMENT

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Numerical simulations and experimental results are presented and compared for the spatiotemporal evolution of an RF argon-silane plasma in which silicon nanoparticles nucleate and grow. The experimental system consisted of a capacitively-coupled parallel-plate system with 13.56 MHz frequency, 4-cm electrode gap, applied RF voltage amplitude of 55 V with measured DC bias at the powered electrode of -20 V, pressure 17 Pa, and gas flow rates of 30 sccm argon and 1 sccm silane introduced through the powered (upper) electrode. Measurements of both plasma light emission and laser light scattering from particles were made as a function of space (axial location between the two electrodes) and time, as particles grow and are transported following the onset of nucleation.

Numerical simulations were based on a previously reported one-dimensional model [1], modified to predict plasma emission and particle light scattering. The same conditions as the experiments were modeled, with the simplification that emission considered only argon, based on a collisional-radiative model. The light scattering simulation calculates Mie scattering from particles, assuming a complex refractive index of 5.0 + 0.1i.

Fig. 1 shows simulation (a) and experimental results (b) for light scattering profiles at several times following the onset of particle nucleation. While there are some discrepancies between the model predictions and the experimental results (e.g. the simulation does not predict the scattering peak near the upper electrode), there are two notable points of agreement. First, particles are pushed toward the lower electrode. This is mainly caused by neutral gas drag due to the convective flow. Second, the peak in scattering intensity that appears near the lower electrode evolves into two spatially separated peaks. The model indicates that this effect is caused by resonances in Mie scattering. Particles near the lower electrode are larger than particles near the center of the electrode gap. A minimum in Mie scattering is predicted for the intermediate-size particles that lie spatially in between.

Reference
PARTICLE SIMULATION OF TRACE SPECIES IN A RAREFIED PLASMA

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The simulation of plasma flows where heavy particles (atoms and ions) are in the rarefied regime requires the solution of Boltzmann-like equations. The most popular kinetic method is the DSMC (direct simulation Monte Carlo) [2] whereby a flow, composed of N_{real} actual particles is modeled by a finite number N_{sim} of macroparticles that each represent a large number W_p (≡ N_{real}/N_{sim}) of real particles. Trace species (species with low N_{real} relative value compared to others) are thus represented by a small number of simulated particles. In the DSMC technique, the properties of each species are obtained by sampling those of the simulated particles over multiple time steps.

The rate of convergence of statistics, \(O\left(1/\sqrt{N_{sim}}\right)\), is thus very low for trace species and hence requires that a large number of time steps be calculated. Some species (such as excited states) that are typically only present in trace amounts, however, play a crucial role in low temperature plasmas and must be accurately simulated. A solution to that dilemma is to increase the number of simulated particles \(N_{sim}\) for the trace species by reducing their weights \(W_p\) and to therefore use different weights between the species [2]. Furthermore, because the relative concentration of species varies spatially due to the effect of diffusion and chemical reactions, the weights further have to vary in space.

A general adaptive procedure for species weights was therefore developed that ensures that all species are simulated by the same number of simulated particles (\(N_{sim}=20\)) in each cell throughout the domain. This in turn allows more accurate statistics to be obtained at greatly reduced computational cost. The adaptive procedure for the weights was applied to a canonical flow of argon gas that was specifically crafted to study the interaction between two different species within the context of a cold ionized rarefied flow. This flow is constituted of two counterflowing jets, as shown in Fig. 1, one composed of ionized Ar gas \((\text{Ar}^+,\text{e}^-)\) and the other of neutral Ar. In future work, the source of neutral Ar will be used to inject metastables in the flow with the aim of shaping the electron energy distribution function of the plasma. Future strategies to simulate electron dynamics within the rarefied gas background will be presented.

References
FAST COMPUTATION OF KINETIC EFFECTS IN PLASMA PROCESSING DISCHARGES

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We conducted 2D PIC simulations of the unstable waves excited in an electronegative (O2) discharge in a two-region plasma with a narrow rf-heated source chamber attached to a wider processing chamber [1]. A double layer forms between the source and processing chambers. Fast and slow waves are excited in the downstream chamber, causing the double layer to “wobble”. Both fluid and kinetic theories of the observed wave excitations were developed and compared with the simulations.

Particle transport in a uniformly magnetized, electronegative (EN) plasma was studied in 2D geometry using a 2D particle-in-cell (PIC) code [2]. The results were compared to analytic one-dimensional (1D) models that approximate the end losses as volume losses. The principal study was the limiting of the transverse electron flow due to strong electron magnetization. The models reasonably approximate the PIC results, and indicate that the cross-field transport is nearly classical.

In a dual frequency sheath, a high frequency uniform sheath motion is coupled with a low frequency Child law sheath motion. The high frequency sheath motion generates most of the electron heating. We showed that for voltage-driven discharges, or discharges driven through a matching network, increasing the low frequency voltage reduces the heating, due to the reduced high frequency current that flows through the sheath [3]. Particle-in-cell (PIC) simulations were used to confirm the voltage-driven result.

We made further improvements to our fast 2D TCP/CCP fluid reactor model [4], built using the commercial finite elements simulation package COMSOL. The simulation consists of an EM model, which solves for both inductive and capacitive fields, a bulk plasma fluid model coupled to an analytic sheath model, and a gas flow model with chlorine feedstock. Simulations of high pressure, highly electronegative discharges have been performed. In addition, we are exploring the E-to-H transition instability seen in previous experiments and global models, and we are assisting in building a similar model for the reactor design of Economou and Donnelly.

Improvements were made to a new user-friendly object oriented code for 1D particle-in-cell (PIC) simulations, used to model argon and oxygen capacitive and inductive discharges. Updated cross section sets for these gases, as well as for xenon, have been incorporated into the code. Simulations of the Ar+ and Xe+ ion velocities near the sheath boundaries in an Ar/Xe discharge have been conducted, using the parameters of the experiment of Lee, Hershkowitz and Severn [5].

References
CONTROLLING PLASMA PROPERTIES IN LOW-COLLISIONAL PLASMAS WITH ACTIVE BOUNDARIES

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PPPL has been conducting experimental and theoretical studies on controlling plasma properties in low collisional plasmas with active boundaries. We have investigated several plasma devices, where energetic electrons and anisotropic electron velocity distribution function (EVDF) are robustly formed and allow control of plasma properties.

The first plasma device is the E×B discharges of the Penning-type at low pressure (10^{-4}-10^{-5} Torr). In such plasma, the electron mean-free path is large compared with the channel width, and the electron velocity distribution function is highly anisotropic. The phenomena of sheath instability and relaxation sheath oscillations are observed and explained due to coupling of the EVDF and sheath properties [1]. Electron emission from biased segmented electrodes is used for controlling the EVDF [2]. Probe and spectroscopic measurements of plasma properties in this discharge were conducted in collaboration with Universities of West Virginia, Wisconsin at Madison and of Houston. In addition to emissive probes and baffled probes [3], we used an advanced probe system developed by University of Michigan. Emissive probe measurements showed that in the presence of a strong electron emission, the floating potential of the emissive wall is 1.5-2.5T_e below the plasma potential [4]. It was also shown that the floating emissive probe is less sensitive to details of the EVDF than floating non-emitting probe. These results, which were obtained for an emissive probe immersed in a low-pressure magnetized xenon plasma, are also relevant to cathodes, plasma thrusters, dusty plasmas, plasma processing, surface discharges and plasma facing components of fusion devices.

The second example is the cathode fall of a regular dc discharge. The cross section of the electron elastic scattering in light gases is relatively small compared with the inelastic cross sections [5] and electrons originated from the cathode do not scatter and form an electron beam moving directly toward anode [6]. The analytical expressions for the EVDF are obtained.

The third device is the dc discharge with a hot cathode and second anode in a form of diaphragm. Application of bias to the diaphragm allows switching the discharge in between two different regimes [7].

References
SIMULATION OF THE EFFECT OF TAILORED BIAS VOLTAGE WAVEFORMS ON THE IED

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The energy of ions bombarding the substrate is critical in plasma etching (and deposition) of thin films, especially when atomic layer precision is required. The ion energy distribution (IED) may be controlled by applying tailored bias voltages on the substrate, or on nearby electrodes immersed in the plasma. A Particle-in-Cell simulation with Monte Carlo Collisions (PIC-MCC) was conducted of the application of tailored DC voltage steps on an electrode, during the afterglow of a capacitively-coupled pulsed argon discharge, to control the energy of ions incident on the counter-electrode. Staircase voltage waveforms with selected amplitudes and durations resulted in ion energy distributions with distinct narrow peaks, having controlled energies and fraction of ions under each peak.

Fig. 1 shows the IED resulting by applying a staircase DC waveform starting at 20 \(\mu\)s into the afterglow (plasma power was pulsed 50 \(\mu\)s ON and 50 \(\mu\)s OFF). In particular, a DC bias of 50 V was applied for 15 \(\mu\)s, followed by 200 V until the end of the afterglow. The gas pressure was 10 mTorr. The IED has four distinct peaks: (1) the peak at \(\sim\)140 eV is due to the plasma ON fraction of the cycle when there is no bias, (2) the peak at very low energies is due to the afterglow when there is no bias. (3) the peak at 50 eV is due to the 50 V DC bias applied during the afterglow, and (4) the peak at 200 eV is due to the 200 V DC bias applied during the afterglow. The locations and intensities of the 50 and 200 eV peaks can be varied by varying DC voltage levels and biasing time windows. The location and intensity of the 140 eV peak can be varied by varying the peak RF voltage and the duty cycle. Temporary electron heating at the moment of application of a DC voltage step did not influence the electron density decay in the afterglow. The IED peaks were “smeared” by collisions, especially at the higher pressures of the range (10-40 mTorr) investigated.

A semi-analytical model was also employed to achieve “designer” IEDs, i.e., distributions with a desired shape and energy spread. This was again accomplished by applying tailored voltage waveforms on the substrate electrode (spike, staircase, judiciously distorted square wave, etc.). Such waveforms could provide, for example, nearly mono-energetic IEDs or other desired shapes. Predicted IEDs were compared with experimental data. Strategies to control the energy flux of bombarding ions or to distribute the total ion energy flux to different energies were identified.

References
The ability to tailor electron energy distribution functions in a controllable manner is a central focus of the DOE funded low-temperature plasma science center (LTPSC). Non-self sustaining “hybrid” plasma discharge generation consisting of a quasi-static bias (direct current or continuous wave) and a superimposed periodic high voltage pulse is a promising way of tailoring a plasma discharge into E/N modes not realized by operating in either mode alone. [1]. The high E/N regime induced by nanosecond length, multi-kilovolt amplitude pulses allows for efficient generation of ion-electron pairs while the lower E/N regime induced by the quasi-static bias channels energy of the electron into specific desired modes of excitation such as molecular dissociation or excitation. Central to realizing the potential of this application is the understanding of the plasma generation process and how this process translates into an efficient reaction.

As part of a collaborative effort focused on nanosecond scale plasma generation, optical and laser based diagnostics are being developed and implemented with the intent of providing validation data to partners developing predictive simulations. In this presentation, diagnostics such as sub-nanosecond resolution two-dimensional phase resolved optical emission spectroscopy (2D PROES) and two-dimensional laser-collision induced fluorescence (2D LCIF) are applied to such plasma discharges are utilized to examine the formation and evolution of plasma in response to high voltages applied across a plasma column. In the context 2D PROES, the evolution of a positive column in generated in 2 Torr of nitrogen gas in response to repetitively applied 20 ns wide, 12 kV amplitude voltage pulse is examined as the pulse repetition rate is varied. The velocity of the wave propagating across the column is obtained from intensity vs time trends presented in figure 1. Comparisons between measured trends and predictive simulations are made. Next, the current status of our implementation of the 2D LCIF technique for the purpose of mapping electron densities before, during and after the application of the high voltage pulse is reported. Limitations placed on helium have spurred the application of the LCIF technique to argon. Finally, we discuss future goals and discuss areas where other collaborative efforts may be formed.

References
Ions, accelerated to high velocities, in the Low Temperature Plasma (LTP) inside Hall Effect Thrusters (HETs) are the thrust-producing constituent. With the continued push for more efficient use of propellant in HETs, time-resolved control of the Electron Energy Distribution Functions (EEDFs) is needed. The ability to tailor the EEDF would allow electrons with energies that contribute to ionization to be increased, and those that do not have enough energy to ionize or that are involved in transient processes to be reduced. However, predictive control of the EEDFs in LTP devices remains a challenging problem in plasma physics due to the complex electromagnetic interactions that take place in the actual system that lead to the turbulent nature of these plasmas. As a first step in addressing the issues involved, initial EEDF measurements were made in a magnetically enhanced, inductively coupled plasma (ICP) with and without the introduction of an axially injected neutral jet stream using a Hiden Langmuir probe (LP) controller along with a lab-built RF compensated LP. Results from the ICP experiments show an increase in low energy electrons when the neutral jet is used (Figure 1). Furthermore, the results reinforced the necessity of moving away from commercial systems to obtain time-resolved data and better current resolution for more accurate EEDFs.

Fig. 1: This figure shows the time-averaged EEDFs as a function of position along the centerline of the cylindrical pyrex tube where the plasma is generated. x=0 in these plots corresponds to 23-cm downstream of the source’s exit plane. The tip of the neutral jet tube is 38-cm from the source. The figure shows an increase in low energy electrons with the neutral argon flow. These EEDFs are non-Maxwellian which is in-line with theory and with other experimental results for partially ionized, low-pressure gas discharge plasmas.[1]

References
Previous experiments[1] have shown that in a low pressure, low temperature plasma, positively biasing an array of thin wires can increase the electron temperature by creating an angular momentum trap to absorb cold electrons. In this experiment, such a device (known as a Maxwell demon) was produced by spot welding 0.025mm tungsten wires onto stainless steel shafts which were then covered with ceramic. This device was used to more than double the plasma electron temperature in the 1eV regime of a multi-dipole chamber operating with mTorr pressures. The Maxwell demon is observed to reduce the cold electron (0.5 - 0.8 eV) population in a plasma with a bi-Maxwellian electron distribution, leaving a single Maxwellian electron distribution of the hot electrons (1.8 – 3 eV). However, at high positive voltages, instabilities in the form of a 50 V potential fluctuation in the kHz frequency range is observed. The instability is associated with higher neutral pressure (> 2mTorr), smaller plasma density and high applied voltage (100 – 150 V). Due to these conditions the instabilities are speculated to be caused by the fluctuation of the effective size of the Maxwell demon through sheath expansion. The Maxwell demon becomes the dominant electrode, which increases the plasma potential, thus its density, and contracts the sheath size, reversing the process. Different Maxwell demon geometries change the instability threshold of applied voltage and neutral pressure despite the total physical surface area of the wires being kept constant. Attempts of taking boxcar-averaged Langmuir probe traces have also been made to understand the instability.

References

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The simulation of plasma flows where heavy particles (atoms and ions) are in the rarefied regime requires the solution of Boltzmann-like equations. The most popular kinetic method is the DSMC (direct simulation Monte Carlo) [1] whereby a flow, composed of \( N_{\text{real}} \) actual particles is modeled by a finite number \( N_{\text{sim}} \) of macroparticles that each represent a large number \( W_p = \frac{N_{\text{real}}}{N_{\text{sim}}} \) of real particles. Trace species (species with low \( N_{\text{real}} \) relative value compared to others) are thus represented by a small number of simulated particles. In the DSMC technique, the properties of each species are obtained by sampling those of the simulated particles over multiple time steps. The rate of convergence of statistics, \( O\left(1/\sqrt{N_{\text{sim}}}\right) \) is however directly linked to the number of particles representing each species. A general adaptive procedure for species weights was therefore developed that ensures that all species are simulated by the same number of simulated particles (\( N_{\text{sim}} \approx 20 \)) in each cell throughout the domain to ensure faster convergence of statistics. The adaptive procedure for the weights was applied to a canonical flow of argon gas that was specifically crafted to study the interaction between two different species within the context of a cold ionized rarefied flow. This flow is constituted of two counterflowing jets, as shown above, one composed of ionized Ar gas \((Ar^+, e^-)\) and the other of neutral Ar.

References
Velocity space diffusion is shown to occur in simulations of E×B devices with strong secondary electron emission (SEE), providing further understanding of phenomena of Relaxation Sheath Oscillations [1] (RSO’s). In a general plasma-wall system, a negative perturbation of the wall potential magnitude $\Phi_c$ allows some previously trapped electrons to overcome the sheath and reach the wall where they are absorbed. Usually, this recharges the wall, canceling the perturbation. But with the presence of strong secondary electron emission (SEE), the extra influx may induce a secondary outflux larger than itself, leading to a net charge loss, amplifying the perturbation as observed in RSO’s.

We identify the precise cause of instability and formulate existence criteria for RSO’s in terms of global plasma parameters. We show the electron diffusion mechanism in phase space is induced by the SEE beams and it has additional implications including energy leaking under broad conditions. The SEE forms peaks in the electron velocity distribution function (EVDF) that make the 1-D x-directed VDF nonmonotonic, causing two-stream instability [2]. This excites plasma waves which perturb particles in velocity space. Bulk particles are driven into the loss region, which leads to a substantial wall flux and sheath instability.

References
DEVELOPMENT OF A VLASOV SOLVER FOR PARTIALLY MAGNETIZED PLASMA

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A partially magnetized plasma such as that generated in a Hall thruster is unsteady, oscillatory and non-equilibrium. In order to obtain accurate results for the non-equilibrium nature of the electrons, the velocity distribution function (VDF) should be taken into consideration by solving the Boltzmann/Vlasov kinetic equations. As a starting point for the development of such a code, a collisionless DC sheath is simulated using an unsteady one-dimensional (1D1V) kinetic solver which discretizes the kinetic equations in both physical and velocity space. Solutions produced using a finite-difference dimensional splitting scheme [2] and a finite-volume unsplit scheme [3] show good agreement with the analytical solution. The unsteady fully-kinetic solver will be extended in future work to collisional plasmas and multi-dimensions.

References

FLUID AND KINETIC SIMULATIONS OF INDUCTIVE/CAPACITIVE ELECTRONEGATIVE DISCHARGES

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We conduct 2D hybrid fluid-analytical and 1D kinetic particle-in-cell (PIC) simulations of highly electronegative inductive/capacitive discharges in order to explore the E to H instability seen in previous global models and experiments. Improvements were made to a previously developed 2D hybrid fluid-analytical TCP reactor model [1], in order to be able to simulate high pressure and highly electronegative discharges. Both inductive and capacitive coupling of the source coils to the plasma are included in the TCP model. A bulk fluid plasma model which solves the time-dependent plasma fluid equations for ion continuity and electron energy balance is coupled with an analytical sheath model and a gas flow model with chlorine feedstock. A 1D planar particle-in-cell code xpdp1 [3] used to simulate capacitive discharges was enhanced to allow inductive heating of the electrons. The exact Maxwell’s equations for the inductive fields were solved for a geometry which consists of a plasma bound between two electrodes with surface currents. A modified oxygen reaction set was used for the PIC simulations in which the attachment cross-section was raised while the recombination cross-section was reduced to achieve a highly electronegative discharge.

Reference
ANALYTICAL APPROXIMATION FOR DIFFERENTIAL CROSS-SECTION OF ELECTRON SCATTERING IN HELIUM FOR MC SIMULATIONS

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Accurate representation of anisotropic scattering in collisions is required for particle simulations of plasmas with energetic (~10^2-10^3 eV) electrons, especially in weakly collisional regimes, for example, for description of a high-voltage dc or rf glow discharge. To simulate the electron kinetics, defined by non-local transport and non-Maxwellian velocity distributions, one needs to correctly reproduce the angular scattering of electrons on neutral atoms within a large energy range.

In numerical simulations, the model of angular scattering should adequately reproduce the macroscopic transport properties and also allow rapid sampling of the probability distribution. This problem is well studied in applications to gases and condensed matter. The most important condition for the model differential cross-section (DCS) is that it should yield the correct value of the transport (momentum-transfer) cross section as a function of electron energy. A screened-Coulomb DCS with energy-dependent screening can be used to match the cross-section data provided by experiment and/or accurate theory, and its integrated probability distribution is easy to invert [1,2].

We present an accurate practical approximation of energy-dependent screening in helium for energies between 0.01 and 1000 eV. The screening is defined by the function \( \xi = \xi(\xi) \) in the DCS:

\[
\frac{1}{\sigma} \frac{d\sigma}{d\Omega} = \frac{1}{4\pi} \frac{1 - \xi^2}{(1 - \xi \cos \theta)^2}.
\]

This function, whose values are between -1 and 1, is implicitly determined by equating the transport cross-section integral to the tabulated values of \( \sigma_{\text{tr}}(\theta) \). For helium, the screening function allows a two-pole rational approximation, with \( x = \sqrt{\xi(\xi)} \) as its argument:

\[
\xi(x) = 1 - \frac{p_1 - p_3 x}{(x - p_1)^2 + p_4} - \frac{p_2 x}{(x - p_5)^2 + p_6}.
\]

The resulting error in the ratio \( \frac{\sigma_{\text{tr}}(\theta)/\sigma_{\text{tot}}(\theta)}{\sigma_{\text{tr}}(\theta)/\sigma_{\text{tot}}(\theta)} \) is under 1%, and the behavior of \((\xi - 1)\) at \( x = \infty \) is in agreement with the cross section given by the Born approximation. Figure 1 shows the comparison of approximated ratio to the one obtained from the reference data.

References:
ION ENERGY DISTRIBUTIONS IN INDUCTIVELY COUPLED PLASMAS HAVING A BOUNDARY ELECTRODE*

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In plasma materials processing there is a continuing need to control the ion energy and angular distribution (IEAD) to surfaces to increasing precision. A relatively recent development in obtaining this control in inductively coupled plasmas (ICPs) is the use of a boundary electrode on which a continuous or pulsed dc bias is applied to the plasma. The scaling of IEADs to a grounded substrate in low pressure (a few to 100 mTorr) ICPs sustained in argon is being numerically investigated using the Hybrid Plasma Equipment Model (HPEM). The electron energy distributions and the IEADs as a function of position and time are obtained using Monte Carlo simulations. Results from the model for Ar plasma densities, electron temperatures, electron distributions and IEADs will be compared to experimental data obtained using a Langmuir probe and a gridded retarding field ion energy analyzer. We found that positive biases provide a nearly linear ability to shift the IEAD in energy by raising the peak in the plasma potential, whereas limited control is afforded with negative biases.

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ETCHING OF α-C:H SURFACE BY ARGON AND HYDROGEN PLASMAS

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A comparative study on etching of the α-C:H film by Ar and H₂ plasmas was performed by using both molecular dynamic (MD) simulation method and in situ ellipsometric measurements during the erosion of thin α-C:H film. The purpose of the study is to establish the role of surface processes in influencing and controlling characteristic plasma distributions functions during the erosion of thin α-C:H film.

The Ar plasma and α-C:H film interaction was studied by performing Ar⁺ impacts on a α-C:H hard film constructed under realistic conditions. We found that the dominant process during Ar⁺ impacts is the depletion of the hydrogen from the α-C:H film, which results in a carbon rich near-surface-region (modified layer). The modified layer thickness increases with increasing ion energy, where its thickness is in a good agreement with experimental results. The H₂ plasma and α-C:H film interaction was studied by performing H₂⁺ impacts on a α-C:H film, as H₂⁺ is one of the major ion species found in the hydrogen plasma. During H₂⁺ impacts onto α-C:H film, the major reactions are found to be: hydrogen insertion, hydrogen depleting and hydrocarbon cluster erosion. The near-surface film structure and composition under steady state conditions is a result of a competition between erosion and insertion processes. We conclude that the modified layer thickness and composition does not depend on the concentration in the initial material. It is dependent on ion (and neutral) flux, energy and composition. The experimental value of the modified layer thickness is found to be bigger than the modeled one. Further studies are performed in order to investigate the cause of the deep surface modification by hydrogen plasma. The effect of H⁺ impacts and synergetic effect of ion and VUV photons will be discussed.
USING PULSED POWER TO CONTROL DISTRIBUTION FUNCTIONS AND ETCH PROPERTIES IN CAPACITIVELY COUPLED PLASMAS

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In capacitively coupled radio frequency (rf) discharges, as used in plasma processing of microelectronic devices, the quality of the etch is directly or indirectly related with the fluxes of radicals and ions to the wafer. Controlling the properties of these fluxes to the wafer can be achieved using pulsed power which provides the possibility of customizing the electron, \(f(\varepsilon)\), and ion, \(f_I(\varepsilon)\), energy distributions. This is particularly the case in multi-frequency capacitively coupled plasmas (CCPs). By pulsing either the low frequency or high frequency one can customize \(f(\varepsilon)\) and \(f_I(\varepsilon)\), as well as the ratio of fluxes of radicals in a manner not otherwise attainable using continuous wave excitation. The choice of duty cycle and pulse repetition frequency (PRF) is important due to the role of thermalization of electrons during the afterglow in determining the cycled average value of \(f(\varepsilon)\) and \(f_I(\varepsilon)\). In addition, charge accumulation in the feature may be controlled by the choice of duty cycle and PRF, subsequently affecting the etch profile. To demonstrate the ability to control feature profiles through control of \(f(\varepsilon)\) and \(f_I(\varepsilon)\) using pulsed plasmas, simulations were performed separately in two regions – on the equipment scale using the Hybrid Plasma Equipment Model (HPEM) and on the feature scale using the Monte Carlo Feature Profile Model (MCFPM). The fluxes of radicals and ions to the wafer in HPEM are transferred to the MCFPM to calculate the etch properties. Plasma properties, \(f(\varepsilon)\) and \(f_I(\varepsilon)\), and ratios of fluxes to the wafer for an Ar/CF\(_4\)/O\(_2\) gas mixture in a 2-frequency CCP will be discussed using results from the HPEM. Etch rates and profiles of SiO\(_2\) resulting from these fluxes will be discussed using results from the MCFPM.

CONTROLLING PLASMA PROPERTIES FOR WOUND TREATMENT WITH A PLASMA JET AND A DIELECTRIC BARRIER DISCHARGE*

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Two approaches are being used in non-thermal atmospheric pressure plasma treatment of human tissue and sterilization of surfaces. In the first, the plasma is produced remotely and its afterglow is delivered in a plume to the tissue. Sterilizing or therapeutic effects are produced by relatively long-lived neutral species and radicals as most of the charged particles do not survive outside the plasma generation region. These jets are usually operated with a few percent of molecular gases such as O\(_2\) in helium to avoid plasma instabilities. In the second approach, plasmas are generated in direct contact with living tissue or bacteria. When dielectric barrier discharges (DBDs) are used for this purpose, the plasma source typically contains the powered electrode while the tissue is the counter electrode [1]. The direct method differs from the indirect technique by delivery of significant fluxes ions and photons to the surface. The treatment of wounds by both methods typically proceeds through a liquid layer covering exposed cells. Control of these sources is required to deliver the desired fluxes of radicals and ions to the surface. In this paper, the interaction between the surface being treated and the atmospheric pressure plasma source will be discussed using results from a computational investigation. Methods to control these sources given changing surface properties will be discussed.

PLASMA-SURFACE INTERACTIONS, EROSION AND IMPACT ON PLASMA DISTRIBUTIONS FUNCTIONS

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The effects of gas mixtures, carbon containing gas, and surface generated carbon (from an a-C:H source) on plasma parameters (T_e, plasma density, EEDF) have been explored with Langmuir probe measurements. We explored mixtures of He with Ar, H_2 with Ar, CH_4 in H_2 and a-C:H erosion in H_2 plasma. Plasma density decreases greatly (10^{11} to 10^9) with only small H_2 or He additions to Ar plasma. The electron temperature also increases with increasing H_2 or He flow. At high H_2 or He flows, the electron energy distribution transitions from Maxwellian distribution to a two energy distribution. The addition of 1-20 % CH_4 into H_2 plasma shows an increase in plasma density and a slight change in the electron temperature. The erosion products of a-C:H films (fluence from the surface calculated from in-situ ellipsometry) in H_2 plasma are volatile hydrocarbons (C_xH_y) and we find that they cause a similar effect on plasma properties as CH_4 addition. This observation could be important for predicting/controlling parameters in plasmas that experience erosion of different hydrocarbon materials (polymers, graphite, etc.).

EXPERIMENTAL STUDY OF FAST IONIZATION WAVE DISCHARGES AT HIGH PULSE REPETITION RATES

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Fast Ionization Wave (FIW) nanosecond pulse discharge propagation in nitrogen, helium, and air is studied experimentally in a rectangular geometry channel / waveguide. A repetitive nanosecond pulse discharge was generated using a custom designed pulsed plasma generator (peak voltage 10-40 kV, pulse duration 30-100 nsec, voltage rise time ~1 kV/nsec, pulse repetition rate up to 40 kHz). In the present experiments, bursts of two alternating polarity discharge pulses are generated at pulse repetition rates ranging from 100 Hz to 40 kHz, at burst repetition rates of 20 Hz. Both positive polarity and negative polarity ionization waves have been studied using a calibrated capacitive probe. Ionization wave speed, as well as time-resolved potential distributions and axial electric field distributions in the FIW discharge are inferred from the capacitive probe data. ICCD images of FIW discharge emission demonstrate that at a low pulse repetition rate (100 Hz), the FIW discharge in helium is diffuse and volume-filling, while the discharge in nitrogen propagates along the walls of the channel. At higher pulse repetition rates, (1 kHz – 40 kHz), the discharge in nitrogen also becomes diffuse. Increasing the pulse repetition rate reduces peak electric field in the ionization wave front. Although at low pulse repetition rates peak electric field in the positive polarity discharge is significantly higher compared to the negative polarity discharge, at high pulse repetition rates electric fields for both discharge polarities become very close.
Numerical and experimental investigations of dusty plasma behavior

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Numerical simulations were performed of a capacitively coupled argon-silane plasma using 1D self-consistent plasma-aerosol model. These simulations were compared to experimental measurements of argon-silane plasma with corresponding operating conditions. Experiments were conducted to measure the spatiotemporal profiles of particle light scattering and plasma emission intensity. It was found both in model and experiments that emission intensity first increases and then decreases. Experimental profiles of particle light scattering exhibit a two peak structure. Similar structure was found in the numerical model. Analysis of numerical results suggests that the two peak structure in numerical model is due to the Mie resonances. Qualitative agreement was found for several major aspects of the evolution of the emission and scattering intensity profiles.
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